

Figure 1

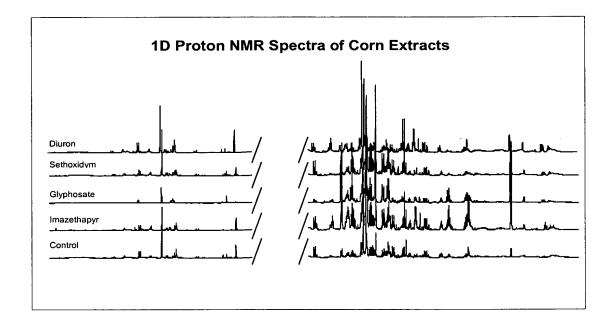


Figure 2

Applicant: Aranibar et al.	
Serial No: Filed Concurrently Herewith	
Aetabolome Profiling Methods Using	Chromatographic and Spectroscopic
attern Recognition Analysis	
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I	2								Output
Training Set			Control	PURSUIT	Sethoxim	Glyphosate	Diuron	Foul	Assignment
na022400 02	2	Control	96666.0	0	0.00001	0.00003	0.00002	0.00001	Control
na022400_05	2	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100 06	53	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100 09	32	Control	0.99998	0	0	0.00001	0.00004	0.00001	Control
na030100 11	졌	PURSUIT	0	0.99996	0.00001	0.00003	0.00004	0.00002	PURSUIT
na030100 14	37	PURSUIT	0	96666.0	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030100_17	4	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030100 19	42	PURSUIT	0	0.99995	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030600 04	21	Control	0.99993	0	0.00002	0.00002	0.00001	0.00001	Control
na030600_08	22	Sethoxydim	0.00002	0.00001	96666.0	0.00005	0.00001	0.00004	Sethoxydim
na030600 10	22	Sethoxydim	0.00002	0.00002	0.99993	0.00002	0.00001	0.00004	Sethoxydim
na030600 13	9	Foul	0	0.00004	0.00002	0	0	0.99991	Foul
na030600 15	62	Glyphosate	0.00007	0.00004	0.00001	0.99992	0	0.00003	Glyphosate
na030600 <sup>7</sup> 16	83	Glyphosate	0.0000	0.00004	0.00003	0.99994	0	0.00003	Glyphosate
na030600 Z0	29	Diuron	0.00004	0.00004	0.00002	0	0.99993	0.00003	Diuron
na030600_21	89	Diuron	0.00007	0.00004	0.00002	0	0.99994	0.00003	Diuron
Test Set									
Ja022400 01	-	Control	0 99998	c	c	0 0000	0.00003	0.00001	Control
na022400_03	- 64	Control	96666 0		0 0000	0.0001	0.00002	0.00001	Control
2022100 00	> <	Control	800000	· c		0 0000	0 00003	0 00001	Control
18022400_04	<b>1</b> (		0.99990			0.0000	0.000	9	Control
1a0zz400_06	9 1	Control	0.99997	<b>-</b>	0.0000			2000	Control
naUZZ4UU_U/	٠,	Control	0.88880	<b>.</b>	0	0.0002	0.00003	0.0000	
na022400_08	œ	Control	0.99997	0	0.00001	0.0000	0.00001	0.0000	
na022400_09	o	PURSUIT	0	0.02733	0	0.01224	0	0.00006	Unknown
na022400_10	우	PURSUIT	0.00086	0.00118	0	0.34361	0	0.00002	Unknown
na022400 11	F	PURSUIT	0.00085	0.00141	0	0.27197	0	0.00002	Unknown
na022400 12	12	PURSUIT	0.00016	0.0025	0	0.12513	0	0.00003	Unknown
na022400 13	5	PURSUIT	0.00013	0.00259	0	0.12979	0	0.00003	Unknown
na022400_14	4	PURSUIT	0.00013	0.00238	0	0.13242	0	0.00003	Unknown
na022400_15	15	PURSUIT	0	0.10029	0	0.00586	0.00001	0.0001	Unknown
na022400_16	9	PURSUIT	0.00005	0.00469	0	0.06222	0	0.00004	Unknown
na022400_17	11	PURSUIT	0.00114	0.00127	0	0.29608	0	0.00002	Unknown
na022400_18	8	PURSUIT	0.00091	0.00139	0	0.27092	0	0.00002	Unknown
na022400_19	19	PURSUIT	0.00048	0.00185	0	0.18992	0	0.00002	Unknown
na022400_20	20	PURSUIT	0.00214	0.00104	0	0.35051	0	0.00002	Unknown
na022400_21	7	PURSUIT	0.00073	0.00088	0	0.34762	0	0.00002	Unknown
na022400_22	22	PURSUIT	0.00046	0.00146	0	0.25479	0	0.00002	Unknown
na022400_23	ន	PURSUIT	0.00086	0.00123	0	0.3072	0	0.00002	Unknown
na030100 01	74	Control	96666.0	0	0	0.00002	0.00005	0.00001	Control
na030100_02	52	Control	0.99997	0	0	0.00001	0.00238	0.00001	Control
na030100_03	8	Control	0.99997	. 0	0	0.00001	0.0000	0.00001	Control
na030100_04	7	Control	00000		0000		, , , ,	•	
		3		=	0.0002	0	00000	0	Contro

Figure 3a

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ata i Recognition Analysis	
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Training Set			Control	PURSUIT	Sethoxim	Glyphosate	Diuron	Foul	Assignment
na030100 07	စ္က	Control	0.99998	0	0	0.00002	0.00002	0.00001	Control
na030100_08	સ	Control	0.99996	0	0.00002	0	0.00001	0.00001	Control
na030100 10	33	PURSUIT	0	96666.0	0.00001	0.00003	0.00005	0.00002	PURSUIT
na030100_12	32	PURSUIT	0	96666.0	0.00001	0.00003	0.00004	0.00002	PURSUIT
na030100 13	99	PURSUIT	0	96666.0	0.00002	0.00004	0.00004	0.00002	PURSUIT
na030100 15	88	PURSUIT	0	0.99994	0.00003	0.00003	0.00005	0.00002	PURSUIT
na030100_16	33	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030100_18	41	PURSUIT	0	0.99995	0.00002	0.00004	0.00004	0.00002	PURSUIT
na030100_20	43	PURSUIT	0	0.9999	0.00005	0.00003	0.00008	0.00003	PURSUIT
na030100_21	44	PURSUIT	0	0.99995	0.00004	0.00004	0.00003	0.00002	PURSUIT
na030100_22	45	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030600_12	29	Sethoxydim	0.00005	0.0003	0.99701	0	0.00003	0.00003	Sethoxydim
na030600 14	61	Glyphosate	0.00006	0.00004	0.00002	0.99994	0	0.00003	Glyphosate
na030600 17	49	Glyphosate	0.00005	0.00005	0.00003	0.99993	0	0.00003	Glyphosate
na030600 18	92	Foul	0	0.00007	0.00003	0	0.00001	0.99993	Foul
na030600_19	99	Diuron	0.00034	0.00003	0.00002	0	0.99992	0.00003	Diuron
na030600_22	69	Diuron	0	0.00005	0.00003	0	0.99989	0.00004	Diuron
na030600_23	2	Diuron	0.00065	0.00014	0.00043	0	0.92715	0.00011	Dinron
na030600_24	7	Diuron	0.00002	0.00005	0.00003	0	0.99993	0.00003	Diuron
Training Set									•
na022400_02	7	Control	0.99996	0	0.00001	0.00003	0.00002	0.00001	Control
na022400_05	2	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100_06	3	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100_09	32	Control	0.99998	0	0	0.00001	0.00004	0.00001	Control
na030100_11	怒	PURSUIT	0	96666.0	0.00001	0.00003	0.00004	0.00002	PURSUIT
na030100_14	37	PURSUIT	0	96666.0	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030100_17	<del>4</del>	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030100_19	45	PURSUIT	0	0.99995	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030600 04	51	Control	0.99993	0	0.00002	0.00002	0.00001	0.00001	Control
na030600_08	22	Sethoxydim	0.00002	0.00001	0.99996	0.00005	0.00001	0.00004	Sethoxydim
na030600_10	24	Sethoxydim	0.00002	0.00002	0.99993	0.00002	0.00001	0.00004	Sethoxydim
na030600 13	9	Foul	0	0.00004	0.00002	0	0	0.99991	Foul
na030600_15	62	Glyphosate	0.00007	0.00004	0.00001	0.99992	0	0.00003	Glyphosate
na030600_16	S	Glyphosate	0.00006	0.00004	0.00003	0.99994	0	0.0003	Glyphosate
na030600_20	29	Diuron	0.00004	0.00004	0.00002	0 (	0.99993	0.00003	Diuron
na030600_21	88	Diuron	0.00007	0.00004	0.0002	0	0.99994	0.00003	Diuron

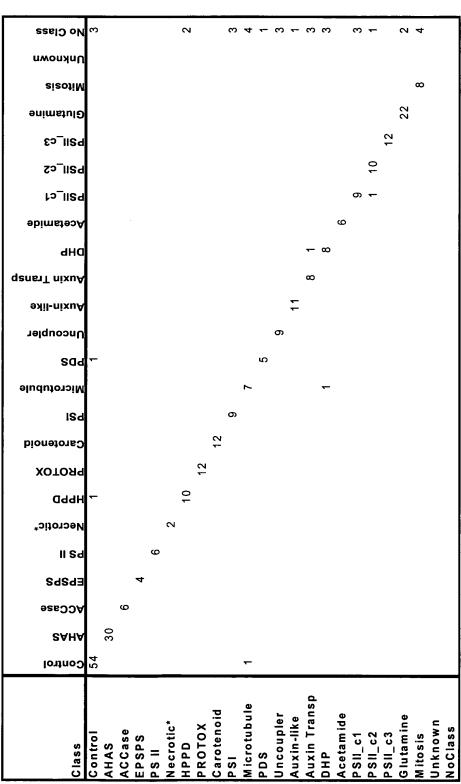
Figure 3b

SNNS result fil	е	V1.4-3D				
Training file		na022400				
Test file na040	400					
No. of patterns	:	24				
No. of input un	its:	1080				
No. of output u	nits:	6				
Startpattern:		1				
Endpattern:		24				
Teaching output	included					
Treatment:	1.1 Contro	1				
Target:	1	0	0	0	0	0
Output:	0.99954	0.00045	0.00001	0.00001	0.00001	0.00001
Treatment:	2.1 Contro	1				
Target:	1	0	0	0	0	0
Output:	0.99936	0.00065	0.00001	0.00001	0.00001	0.00001
Treatment:	3.1 Contro	1	.=			
Target:	1	0	0	0	0	0
Output:	0.99951	0.00047	0.00001	0.00001	0.00001	0.00001
Treatment:	4.1 Contro	1		·		
Target:	1	_ 0	0	0	0	0
Output:	0.99963	0.00037	0.00001	0.00001	0.00001	0.00001
Treatment:	5.1 Chlors				-	
Target:	0	0	0	0	0	0
Output:	0.00159	0.99843	0	0.00001	0	Ö
Treatment:	6.1 Chlors				<del></del>	
Target:	0	0	0	0	0	0
Output:	0.00806	0.99165	0	0	0	0
Treatment:	7.1 Chlors					
Target:	0	0	0	0 .	0	0
Output:	0.00334	0.99669	0	0	0	0
Treatment:	8.1 Chlors					
Target:	0	0	0	0	0	0
Output:	0.00014	0.99985	Ō	0.00001	0	0
Treatment:	9.1 Chlors					
Target:	0	0	0	0	0	0
Output:	0.00667	0.99376	Ö	0	Ö	ŏ
Treatment:	10.1 Imaza		<del>-</del>		· · · · · · · · · · · · · · · · · · ·	
Target:	0	0	0	0	0	0
Output:	0.00044	0.99955	0	0	Ö	Ö
Treatment:	11.1 Imaza					
Target:	0	0	0	0	0	0
Output:	0.00013	0.99987	Õ	0	0	0
Treatment:	12.1 Imaza				<del>-</del>	-
Target:	0	0	0	0	0	0
Output:	0.00208	0.99798	0	0.00001	0.00001	o l
Jucpuc.	1 3.00200	0.22,20		U.0000±	0.0001	

Figure 4a

SNNS result fil	е	V1.4-3D				
Training file		na022400				
Test file na040	400					
No. of patterns	:	24				
No. of input un	its:	1080				
No. of output u		6				
Startpattern:		1				
Endpattern:		24				
Teaching output	included					
Treatment:	13.1 Imaza	methabenz				
Target:	0	0	0	0	0	0
Output:	0.00223	0.99755	0	0	0	0
Treatment:	14.1 Imaza	methabenz				
Target:	О	0	0	0	0	0
Output:	0.06789	0.93484	0	0	0	0
Treatment:	15.1 Sulfu	meturon				
Target:	0	0	0	0	0	0
Output:	0.00046	0.99955	0	0	0	0
Treatment:	16.1 Sulfu	meturon				
Target:	0	0	0	0	0	0
Output:	0.00102	0.999	0	0.00001	0	0
Treatment:	17.1 Sulfu					
Target:	0	0	0	0	0	0
Output:	0.00194	0.99813	0	0.00001	Ö	0
Treatment:	18.1 Sulfu			0.100002		
Target:	0	0	0	0	0	0
Output:	0.00013	0.99987	Ö	Ö	0	0
Treatment:	19.1 Sulfu					<u>-</u>
Target:	0	0	0	0	0	0
Output:	0.00014	0.99985	Ö	0	0	Ō
Treatment:	20.1 Imaza					-
Target:	0	0	0	0	0	0
Output:	0.0018	0.998	0	0	0	0
Treatment:	21.1 Imaza	<del></del>	<del> </del>	<del>-</del>		
Target:	0	0	0	0	0	0
Output:	0.00031	0.99968	0	0.00001	0	0
Treatment:	22.1 Imaza		. <del></del>			
Target:	0	0	0	0	0	0
Output:	0.00175	0.99791	0	Ö	Ö	Ö
Treatment:	23.1 Imaza				<del>-</del>	
Target:	0	0	0	0	0	0
Output:	0.00018	0.9998	0	0	0	0
Treatment:	24.1 Imaza				<del>-</del>	<u> </u>
Target:	0	O DAT	0	0	0	0
Output:	0.06579	0.93074	0	0	0	0
output.	10.00575	0.93074	<u> </u>	•	U	<u> </u>

Figure 4b



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Serial No: Filed Concurrently Herewith

tabolome Profiling Methods Using Chromatographic and Spectroscopic tern Recognition Analysis 6. 16313-0089 Sheet 7 of 10

Rows: Teaching Input; Columns: Classification for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

Figure 5

Applicant: Aranibar et al.

Serial No: Filed Concurrently Herewith
etabolome Profiling Methods Using Chromatographic and Spectroscopic
httern Recognition Analysis

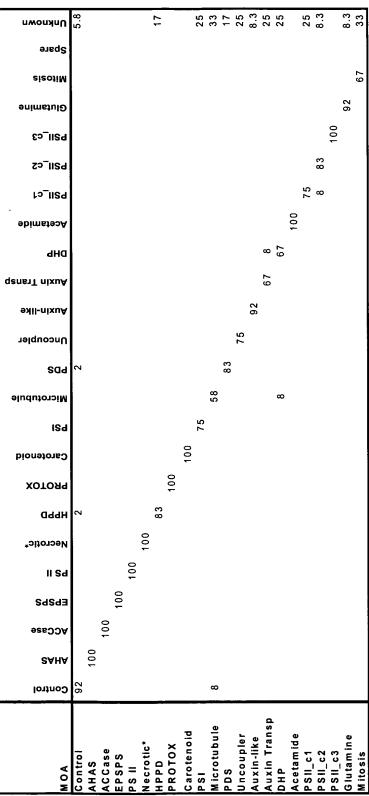
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stnald #	31	17	2	7	0	_	9	9	9	9	9	ж	9	9	9	9	<u>س</u>	9	2	9	12	9	0	0
	2 3	0	0	0	0	0	3	0	0	2	⊢	┢		<del>                                     </del>	Ͱ	-		╂─	-	⊢	-	┢	┿	-
Опкломп	├—	┢	╁	1	╁	├-	╁─				4	2	匚	2	7	5	F	7	F	0	0	3	0	0
Spare	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SisotiM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	ω	0	0
Glutamine	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Ξ	0	0	0
E5_II29	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9	0	0	0	0
PSII_c2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-	∞	0	0	0	0	0
PSII_c1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	ς.	-	0	0	0	0	0
Acetamide	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
рнь	0	0	0	0	0	0	0	0	0	0	0	0	-	0	-	-	0	0	0	0	0	0	0	0
qenrıT nixuA	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0
Auxin-like	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0
Uncoupler	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0
PDS	-	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
Microtubule	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0
ISA	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Carotenoid	0	0	0	0	0	0	0	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
хотояч	0	0	0	0	0	0	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ПФРБ	1	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Necrotic*	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Not Used	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
EPSPS	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ACCase	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SAHA	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Control	27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
CLASS	Control	AHAS	ACCase	EPSPS	Not Used	Necrotic*	HPPD	PROTOX	Carotenoid	ISd	Microtubule	PDS	Uncoupler	Auxin-like	Auxin Transp	DHP	Acetamide	PSII_c1	PSII_c2	PSII_c3	Glutamine	Mitosis	Spare	NoClass

Rows: Teaching Input; Columns: Classifications for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

Figure 6





Necrotic = dead or decaying plant

Rows: Teaching Input, Columns: Classification as Percentage of Total Plants Tested for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

Figure 7



Пикпомп	9	Т	Τ	T	Т	T	20		Τ	33	29	19	17	33	33	83	33	33	2	T	Г	20
Spare	1-	+	+	-		+	1		-	<del>                                     </del>			F	-		+	6,	F.	┼	-		S
sisotiM	1	t	1	$\vdash$	+	1		<del> </del>	-	+	-			-		-	ļ <u>.</u>	-	-			20
Glutamine	1	$\vdash$	+-	-	$\dagger$		+	-			+	-	+	-			-	-			92	100
E5_IIS9	Ħ	-	Ť	+	<u> </u>	-	-			$\vdash$	-	$\vdash$	$\dagger$		-	-	-		-	001	5	├
22_112q		<del> </del>	<del> </del>		-	+			-	<u> </u>	-	+-	-			-	-	17	∞	=	-	-
15_H24	╁╴	1	-	+		1			-		-		-			-	+-	20	2	-		
Acetamide	-	-		-	-				-	$\vdash$	-		-			-	19	-	-	<u> </u>	ļ	
т		-		-		-		$\vdash$	$\vdash$	-		<u> </u>	77	-	17	17	-	-			-	$\vdash$
Auxin Transp	<del> </del>	-					$\vdash$				<del> </del>	$\vdash$			20	╁═╴						
Auxin-like	<del> </del>	$\vdash$		-	+	1	-					-		19	<u>σ</u>	-		ŀ			_	
Uncoupler			-		-	-	-	-		-	-	-	29			-						
-	3	<u> </u>	-		<del>                                     </del>	-				-	-	33	9			-		-				
Microtubule		-	<u> </u>	<u> </u>	1			-	-	-	33	<u></u>						_	-	-		
	-		-	-		-	-	-		29	<u>.</u>	-				+						
Carotenoid PSI				$\vdash$		-			001	9		-				-					_	
	-	-	-			-	-	901	Ĭ <u> </u>	-			-			-		_				_
ХОТОЯЧ	3		_			-	20	=								+						
Necrotic*		-		ļ		100	4,	_			_			_		+						
	_	-		-		-		_			_					-						
Not Used		-		901	_			_								+						_
EPSPS		-	100	=	-						ļ					-						_
ACCase		901	<u> </u>							_					•	-						_
SVHV	28	=																			-	
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Class	_	S			_										<u>п</u> о	P 15	le 16	1 17	2 18		29 19	is 21
	Contro]	<b>AHAS</b>	<b>ACCase</b>	EPSPS	Not Used	Necrotic*	HPPD	PROTOX	Carotenoid	PSI	lpal	PDS	Uncoupler	Auxin-like	Auxin Fransp	DHP	Acetamide	II c1	PSII c2	PSII c3	Glutamine	Mitosis
SS	ಶ	V	AC	E	Not	lecr	$ \Pi $	RO	rote		roti		1001	ixi	▼ L		eta	PSII	PS	PS	uta	Ξ
CLASS								Ы	Ca		Microtubule		i S	A			Ψ				ਠ	

Rows: Teaching Input, Columns: Classification as Percentage of Total Plants Tested for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, I "Spare" Class, and "Unknown" Added by SNNS)

## Figure 8